A ‘Non-Parametric’ Version of the Naive Bayes Classifier

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Abstract

Many algorithms have been proposed for the machine learning task of classification. One of the simplest methods, the naive Bayes classifier, has often been found to give good performance despite the fact that its underlying assumptions (of independence and a Normal distribution of the variables) are perhaps violated. In previous work, we applied naive Bayes and other standard algorithms to a breast cancer database from Nottingham City Hospital in which the variables are highly non-Normal and found that the algorithm performed well when predicting a class that had been derived from the same data. However, when we then applied naive Bayes to predict an alternative clinical variable, it performed much worse than other techniques. This motivated us to propose an alternative method, based on naive Bayes, which removes the requirement for the variables to be Normally distributed, but retains the essential structure and other underlying assumptions of the method. We tested our novel algorithm on our breast cancer data and on three UCI datasets which also exhibited strong violations of Normality. We found our algorithm outperformed naive Bayes in all four cases and outperformed multinomial logistic regression (MLR) in two cases. We conclude that our method offers a competitive alternative to MLR and naive Bayes when dealing with data sets in which non-Normal distributions are observed.

Key words: supervised learning, naive Bayes, logistic regression, breast cancer, UCI data sets

1. Introduction

Worldwide, breast cancer is the second most common type of cancer and the fifth most common cause of cancer death. This disease poses a serious threat for women’s health. Since the early years of cancer research, biologists have used the traditional microscopic technique to assess tumour behavior for breast cancer patients. Precise prediction of tumours is critically important for the diagnosis and treatment of

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Preprint submitted to Knowledge-Based Systems *February 17, 2011*

cancer. Modern machine learning techniques are progressively being used by biologists to obtain proper tumour information from the databases. Among the existing techniques, supervised learning methods are the most popular in cancer diagnosis [1].

Many supervised classification algorithms have been proposed in literature, from decision trees to neural networks, from support vector machines to Bayesian classifiers. The naive Bayes classifier continues to be a popular learning algorithm for data mining applications due to its simplicity and linear run-time [2]. It is a fast-supervised classification technique which is suitable for large-scale prediction and classification tasks on complex and incomplete data sets. Naive Bayesian classification assumes that the variables are independent given the classes. The naive Bayes classifier applies to learning tasks where each instance x is described by a conjunction of attribute values and where the target function $f(x)$ can take on any value from same finite set V [3]. This classifier is based on another common simplifying assumption: the values of numeric attributes are normally distributed within each class. On many real-world data sets, as in those presented in this paper, the latter condition is strongly violated. It might happen that, even in such a situation, the naive Bayes classifier performs well, but one should always be aware that not all the hypotheses are satisfied.

According to John and Langley [4], methods for inducing probabilistic descriptions from training data have emerged as a major alternative to more established approaches to machine learning, such as decision-tree induction and neural networks. However, some of the most impressive results to date have come from a much simpler – and much older – approach to probabilistic induction such as the naive Bayesian classifier [4]. Despite the simplifying assumptions that underlie the naive Bayesian classifier, experiments on real-world data have repeatedly shown it to be competitive with much more sophisticated induction algorithms. Furthermore, naive Bayes can deal with a large number of variables and large data sets, and it handles both discrete and continuous attribute variables. In [4] the assumption that data are generated by a single Gaussian distribution is abandoned because it is not always the best approximation. Authors suggest to investigate more general methods for density estimation, introducing what they call "Flexible Bayes", an extension of the naive Bayes classifier which uses a kernel density estimation. This method is very similar to the naive Bayes, but the density of each continuous variable is estimated averaging over a large set of kernels. The method performs well in domains that violated the normality assumption and, in general, this flexible Bayesian classifier generalizes better than the version that assumes a single Gaussian.

Bouckaert [5] also assesses that naive Bayes classifiers perform well over a wide range of classification problems, and, compared with more sophisticated schemes, they often perform better. He proposes a comparison of the three main methods for dealing with continuous variables in naive Bayes classifiers, namely the normal method, the kernel method and discretization. The normal method is the classical method that approximates the distribution of the continuous variable using a Gaussian distribution. The kernel method is the one cited above [4] which uses a non-parametric approximation. Finally, the discretization method [6] first discretizes the continuous variables into discrete ones, leaving a simpler problem without any continuous variable. In general, it is acknowledged that the normal method tends to perform worse than the other two methods. However, according to the simulations and experiments run by Bouckaert, none of the three methods systematically outperforms the others on all problems that were considered.

Much recent work has focussed on the accuracy of the naive Bayes classifier, proposing new alterations to the technique to improve its performance. Yager [7] provides an extension of the classifier in a manner that gives the user more parameters for matching data. In particular, a version of naive Bayes is proposed which involves a weighted summation of products of probabilities.

Hall [2] states that many enhancements to the basic naive Bayes algorithm have been proposed to help mitigate its primary weakness - the assumption that attributes are independent given the class. He proposes a simple filter method for setting attribute weights to improve its performance without degrading the quality of the model. He also considered training time, in that normal naive Bayes algorithm is linear in both the number of instances and attributes, and his proposed method is supposed to maintain the run-time complexity and the simplicity of the final model.

According to Lee [8], a different approach to improve the performance of the naive Bayes is to include unlabeled data as part of the training data in certain problems. Most classic methods of learning with unlabeled data use a generative model for the classifier and use an Expectation-Maximisation method [9]. Lee's approach first calculates the estimates of parameters using only labeled data. After acquiring estimated values of parameters, the algorithm classifies unlabeled data. After the class values of each unlabeled data are calculated, the algorithm is trained again using both originally labeled data and formerly unlabeled data. The algorithm iterates this process until there is no or very little change in the estimated target values of the unlabeled data [8]. Hsu et al. [10] examine the problem of mixed data, stating that the naive Bayes method is inapplicable when dealing with such data. They propose to use the Extended Naive Bayes and demonstrate its efficiency in comparison with other classification algorithms.

Many actual data sets are often incomplete for various reasons but most of the supervised learning techniques deal with complete data. According to Chen and colleagues [11] methods of constructing classifiers for incomplete data deserve more attention. Classifiers such as naive Bayes classifiers and C4.5 often adopt two simple strategies to deal with incomplete data: to ignore the instances with unknown entries or to ascribe these unknown entries to a specified dummy value of the respective attribute variables. To overcome these limitations, a selective Robust Bayes Classifier for incomplete data based on gain ratio was proposed [11]. The method needs no assumption about the missing data mechanism and, when tested over 12 benchmark incomplete data sets, showed an improvement in the accuracy of classification with respect to the normal naive Bayes.

More recently, Balamurugan et al. proposed a method to handle the situation where there is an equal probability for the class label value, i.e. when the training data satisfy the constraint that the probability of every class label attribute is evenly distributed among the distinct attribute values [12]. When this happens, the naive Bayes classifier fails to classify the record correctly due to the random assignment of class labels. The approach proposed has been named 'NB+', and it aims to suggest a solution with the help of a partial matching method. The validation of NB+ over 18 public data sets chosen from the UCI machine learning repository [13] shows a higher degree of accuracy than the traditional naive Bayes algorithm.

Despite the number of approaches proposed for improving the naive Bayes performance, it seems that a specific criterion for handling non-Normal, continuous and complete data has not been suggested yet. In this paper, we present a new method for the implementation of a Bayesian classifier dealing with continuous variables which, as in our cases, do not follow Normal distributions (see Fig. 1). The motivation for this new algorithm comes from a previous study [14], in which we reviewed three different supervised learning techniques and found that the naive Bayes gave the most reliable results although variables were not following a Normal distribution. In our breast cancer dataset, the variables have distributions that are very far from Normal and, further, there is no obvious way in which they could be transformed to Normal. Our approach has the same structure as the naive Bayes one, considering the ratio between areas under the variables' distribution curves. We compare our new method with both the original naive Bayes algorithm and a multinomial Logistic Regression model. We aim to show that the new 'non-parametric' classifier outperforms the other two methods or at least is more accurate than the traditional naive Bayes. For our analysis, a novel dataset on breast cancer [15] and three case series from the UCI Machine Learning Repository [16, 13] were considered.

[Figure 1 about here.]

The paper is structured as follows. In Section 2, a review of the naive Bayes classifier and its relation with Logistic Regression are reported. Section 3 describes our new method. Then, in Section 4, the data sets used for our experiments are presented together with measures for assessing and predicting the accuracy. Results obtained by the different classifiers are shown in Section 5. Sections 6 and 7, respectively, highlight the main contributions of this work and discuss the results.

2. Existing Methods

2.1. Naive Bayes Classifier

A naive Bayes classifier is a simple probabilistic classifier based on applying Bayes' theorem with strong independence assumptions. Let C be the random variable denoting the class of an instance and X be a vector of random variables denoting the observed attribute values. Let c be a particular class label and x represent a particular observed attribute value. According to the independence assumption, attributes $X_1 \dots X_n$ are all conditionally independent of one another, given C. The value of this assumption is that it dramatically simplifies the representation of the conditional probability $P(X|C)$, and the problem of estimating it from the training data [17]. In fact, accurately estimating $P(X|C)$ typically requires many examples. To see why, let us consider the number of parameters we must estimate when C is boolean and X is a vector of n boolean attributes. In this case, the following set of parameters should be estimated:

$$\theta_{ij} \equiv P(X = x_i | C = c_j)$$

where the index i takes on 2^n possible values (one for each of the possible vector values of X), and j takes on 2 possible values. Therefore, approximately 2^{n+1} parameters need to be estimated. To calculate the exact number of required parameters, note for any fixed j, the sum over i of θ_{ij} must be one. Therefore, for any particular value c_j, and the 2^n possible values of x_i, we need compute only $2^n - 1$ independent parameters. Given the two possible values for C we must estimate a total of $2(2^n - 1)$ such θ_{ij} parameters for learning Bayesian classifiers [17]. The Naive Bayes classifier, instead, reduces this complexity by making a conditional independence assumption that reduces the number of parameters to be estimated, when modeling $P(X|C)$, form the original $2(2^n - 1)$ to just $2n$. Moreover, to estimate $P(C|X)$, the training data can be used to learn estimates of $P(X|C)$ and $P(C)$. New X examples can then be classified using these estimated probability distributions, plus Bayes rule. This type of classifier is called a *generative* classifier, because the distribution $P(X|C)$ can be viewed as describing how to generate random instances X conditioned on the target attribute C [17].

If we have a test case x to classify, the probability of each class given the vector of observed values for the predictive attributes may be obtained using the Bayes' theorem:

$$p(C = c | X = x) = \frac{p(C = c)p(X = x | C = c)}{p(X = x)}$$

and then predicting the most probable class. Because the event is a conjunction of attribute values assignments, and because of the attributes conditional independence assumption, the following equation may be written:

$$p(X = x | C = c) = \prod_i p(X_i = x_i | C = c)$$

which is quite simple to calculate for training and test data [4].

A standard assumption is that, within each class, the values of numeric attributes are normally distributed. One can represent such a distribution in terms of its mean and standard deviation, and the probability of an observed value from such estimates can be computed. For continuous attributes we can write the probability density function for a normal (or Gaussian) distribution as [4]

$$g(x; \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}. \tag{1}$$

The traditional naive Bayes classifier is still widely used as a popular learning algorithm for data mining applications due to its simplicity [2]. However, we should be aware that many real-world problems are represented by data which often do not satisfy all the assumptions of this technique. To overcome the non-independence of variables given the class, many techniques have been developed in the past [18]. In this paper, we are interested in developing a new algorithm which reflects the structure of the naive Bayes, but that is also able to handle continuous and non-normal data. Solutions like the one proposed by Hsu and colleagues [10], for example, are then not suitable for our problem, because we are not interested in dealing with mixed data sets.

2.2. Logistic Regression

Logistic Regression is an approach to learning functions of the form $f : X \rightarrow C$, or $P(C|X)$ in the case where C is discrete-valued, and $X = \langle X_1 \ldots X_n \rangle$ is any vector containing discrete or continuous variables [17]. Logistic Regression assumes a parametric form for the distribution $P(C|X)$, then directly estimates its parameters from the training data. In this way, the 'two-steps' approach for estimating $P(C|X)$ used by the naive Bayes may be overtaken. In this sense, Logistic Regression is often referred to as a *discriminative* classifier, because we can view the distribution $P(C|X)$ as directly discriminating the value of the target C for any given instance X. As shown in [17], if C is boolean and the Gaussian Naive Bayes (GNB) assumptions hold, then asymptotically (as the number of training examples grows toward infinity) the GNB and Logistic Regression converge toward identical classifiers. However, as demonstrated in detail in [19], GNB parameter estimates converge toward their asymptotic values in order $\log n$ examples, where n is the dimension of X. In contrast, Logistic Regression parameter estimates converge more slowly, requiring order n examples.

When the response variable C is boolean (0 or 1), the Logistic Regression, fitted by a generalised linear model (GLM), may be used to model $P(1|X)$; a multinomial logistic regression (MLR) model is instead needed when there are more than two classes.

3. A 'Non-Parametric' Bayesian Classifier

In a previous study [14], three different classification techniques (C4.5 decision tree classifier, Multi-Layer Perceptron artificial neural network and the naive Bayes classifier) were reviewed and it was found that the naive Bayes gave the most reliable results even though its simplifying assumptions were strongly violated by the data analysed. We then thought of developing a new algorithm with the same 'structure' of the naive Bayes, but that could be used with numerical non-normal data. Like the traditional naive Bayesian classifier, the new algorithm should be a 'white-box' model, in which the reason for arriving at the classification can be explicitly determined by examining the model itself. We were then not interested in using Neural Networks or Support Vector Machines to replace the naive Bayes because the former are 'black-box' models, while the latter can be only used in problems with two classes output.

The main idea of our new algorithm is that the closer a variable value is to its median in a particular class, the higher is the probability to be assigned to that specific group. This is similar to the traditional naive Bayes, where the mean is used instead of the median.

At the beginning of the algorithm we computed the median value of each feature in every class and the *priors* probabilities, which were defined as the ratio between each class size (in terms of number of data points) and the total number of cases.

The following step is the main part of our method in which the single probabilities are calculated.

For each variable, we check whether the single variables' values are smaller or bigger than the median of that variable distribution in each class. If the value is smaller, we calculate the area under the histogram which remains on the left with respect to the value being analysed (Fig. 2A). If the amount is bigger, the area on the right side is computed, taking in consideration the portion of the histogram delimited by the value and the maximum (Fig. 2B). The amount returned is then divided by half of the total observations, as we assume that the total area under the histogram is equal to one.

[Figure 2 about here.]

In the next step, for each patient and each class, we compute the product of all the features probabilities times the *priors*.

$$p[i,k] = priors[k] \times \prod_{j=1}^{p} prob[j,k] \quad \text{for } k = 1,\dots,K$$

where j runs over the p variables, i represents patients and K is the number of groups.

The final step of our algorithm is the calculation of the prediction for each instance: it is defined as the class number which gives the highest $p[i,k]$ ($\arg\max_k p[i,k]$).

With a little abuse of notation, we can summarise our algorithm in the following way: calling m, min and max the median, minimum and maximum values of each feature in each class, we want to find k for which $p[i,k]$ is maximised, where

$$p[i,k] = priors[k] \times \begin{cases} \prod_j \frac{1}{N/2} \int_{min}^{x} g(x;m) & x < m \\ \prod_j \frac{1}{N/2} \int_{x}^{max} g(x;m) & x > m \\ 1 & x = m \end{cases},$$

and j represents one of the features, x is the particular variable's value under investigation and i runs over the instances set. For similarity with the naive Bayes (see Equation 1), we call $g(x,m)$ the function that represents each variable distribution, even though it is not always possible to express it in an explicit form. However, the overall 'structure' of our new algorithm reflects the one of the traditional naive Bayes.

4. Experimental Settings

For our experiments, the WEKA software [20] was used to run the naive Bayes classifier. It is a popular suite of machine learning free software written in Java and developed at the University of Waikato in New Zealand. Logistic regression and our new method were run using R, a free software environment for statistical computing and graphics [21]. All the classification techniques require a reasonable computational time, especially if compared with neural networks or SVMs [22]. In particular, for the traditional naive Bayes and for our 'non-parametric' Bayesian classifier, the training time is linear in both the number of instances and attributes [2].

In the next two subsections, the data sets analysed in this study are presented.

4.1. The Nottingham Breast Cancer Data Set

In a previous study [15], immunohistochemistry techniques applied to tissue microarray (TMA) preparations of 1,076 cases of invasive breast cancer were used to study the combined protein expression profiles of a large panel of 25 well-characterized biomarkers (reported in Table II of [15]) related to epithelial cell lineage, differentiation, hormone and growth factor receptors and gene products known to be altered in some forms of breast cancer. Most of the proteins selected have a well-established role in breast carcinogenesis. In addition, the gene transcripts of these proteins have been reported to be important candidate discriminator genes in stratifying breast cancer into distinct groups based on previous cDNA microarray studies [23, 24, 25, 26, 27, 28].

Several clinical information were also available in this data set, including the Nottingham Prognostic Index (NPI) score and its defining factors (tumour size, grade, and stage of disease). The NPI was defined in [29] as a prognostic index which may be used to categorise patients affected by breast cancer according to its value. In particular, the index is calculated according to the following formula:

$$NPI\ Score = (0.2 \times size) + grade + stage$$

and five different groups may be defined depending on its value (see Table 1). We used the 25 biomarkers to predict the NPI groups.

[Table 1 about here.]

4.2. UCI Machine Learning Repository Data Sets

The other datasets we used to validate our new method are taken from the UCI machine learning repository [13]: `vehicle, glass,` and `haberman`.

For the `vehicle` dataset, the purpose is to classify a given silhouette as one of four types of vehicle, using a set of features extracted from the silhouette. Each vehicle may be viewed from one of many different angles. The original purpose was to find a method of distinguishing 3D objects within a 2D image by application of an ensemble of shape feature extractors to the 2D silhouettes of the objects. Measures of shape features extracted from example silhouettes of objects to be discriminated were used to generate a classification rule tree by means of computer induction. This object recognition strategy was successfully used to discriminate between silhouettes of model cars, vans and buses viewed from constrained elevation but all angles of rotation. The features were extracted from the silhouettes by the HIPS (Hierarchical Image Processing System), which extracts a combination of scale independent features utilising both classical moments based measures such as scaled variance, skewness and kurtosis about the major/minor axes and heuristic measures such as hollows, circularity, rectangularity and compactness. Four 'Corgie' model vehicles were used for the experiment: a double decker bus, Cheverolet van, Saab 9000 and an Opel Manta 400. This particular combination of vehicles was chosen with the expectation that the bus, van and either one of the cars would be readily distinguishable, but it would be more difficult to distinguish between the cars [16].

The `glass` dataset is taken from the USA Forensic Science Service and six types of glass, defined in terms of their oxide content (i.e. Na, Fe, K, etc), are considered. The study of classification of types of glass was motivated by criminological investigation: at the scene of the crime, the glass left can be used as evidence, if it is correctly identified [30, 13].

The `haberman` dataset contains cases from study conducted between 1958 and 1970 at the University of Chicago's Billings Hospital on the survival of patients who had undergone surgery for breast cancer [31, 13].

Table 2 provides a summary of the `breast cancer` and the three UCI benchmark datasets. Each variable in each dataset was tested for normality using the Shapiro test [32]. Since no test data sets were provided in the benchmark sets, we used ten-fold cross validation to evaluate the performance of our algorithm. That is, each dataset was split randomly into ten subsets and one of those sets was reserved as a test set; this process was repeated ten times.

[Table 2 about here.]

Since two of the UCI datasets (namely `vehicle` and `glass`) had been also analysed by Bouckaert [5], comparing three main methods for dealing with continuous variables in naive Bayes classifiers, a comparison with Bouckaert's results will be performed simply by looking at the average accuracies reported in the original work [5]. As a matter of fact, in [5], the kernel method and the discretisation one have been used in comparison with the original naive Bayes.

4.3. Measures for Assessing and Comparing Performance

There are many different measures for predicting the accuracy of a model [33]; two of them are *calibration* and *discrimination.* When a fraction of about P of the events we predict with probability P actually occur, it can be said that the predicted probabilities are well calibrated and a suitable model for $P(C|X)$ has been found [34]. Discrimination, instead, measures a predictor's ability to separate patients with different responses [33]. When the outcome variable is dichotomous and predictions are stated as probabilities that an event will occur, calibration and discrimination are more informative than other indices (like, for example, the expected squared error) in measuring accuracy [33]. Calibration plot is a method that shows how well the classifier is calibrated and a perfectly calibrated classifier is represented by a diagonal on the graph [35]. In this work, these plots were produced following the procedure described in [34], plotting the fitted values versus the actual average values.

A c (for *concordance*) index is a widely applicable measure of predictive discrimination and it applies to ordinary continuous outcomes, dichotomous diagnostic outcomes and ordinal outcomes. This index of predictive discrimination is related to a rank correlation between predicted and observed outcomes. The c index is defined as the proportion of all usable patient pairs in which the predictions and outcomes are concordant. For predicting binary outcomes, like in the `haberman` survival dataset, c is identical to the area under a receiver operating characteristic (ROC) curve [33].

A ROC curve is a tool to measure the quality of a binary classifier independently from the variation in time of the ratio between positive and negative events [35]. In other words, it is a graphical plot of the *sensitivity* versus *(1 - specificity)* for a binary classifier system as its discrimination threshold is varied. The ROC can also be represented equivalently by plotting the fraction of true positives (TPR = true positive rate) versus the fraction of false positives (FPR = false positive rate). A completely random guess would give a point along a diagonal line (the so-called line of no-discrimination) from the left bottom to the top right corners. Usually, one is interested in the area under the ROC curve, which gives the probability that a classifier will rank a randomly chosen positive instance higher than a randomly chosen negative one. A random classifier has an area of 0.5, while an ideal one has an area of 1.

The accuracies of the obtained classifications were evaluated for all techniques simply by looking at the percentage of the correctly classified instances.

In the following, the acronyms NB (naive Bayes) and NPBC (non-parametric Bayesian classifier) will be used to indicate, respectively, the usual naive Bayes classifier and our new method. MLR will stay for Multinomial Logistic Regression, while GLM for Generalised Linear Model.

5. Experimental Results

First of all, we deleted from the `breast cancer` data four cases for which the NPI value was missing. Then, we started our experiments running the naive Bayes classifier in WEKA using the 10-fold cross validation option. Also when using our new method in R, the 10-fold cross validation option was utilised.

We found, for the `breast cancer` dataset, that only 249 (23.2%) patients were correctly assigned to their particular class, while the remaining 823 (76.8%) were misclassified. For the Statlog `vehicle` dataset, instead, naive Bayes properly classified 381 instances (45.0% of the total amount), leaving 465 cases (55.0%) incorrectly assigned to their group. When considering the glass dataset, the algorithm correctly classified almost just half of the cases (48.6% which corresponds to 104 data points), leaving the other half (110 cases, equal to 51.4%) not properly classified. For the last dataset analysed (haberman), naive Bayes assigned 229 patients (74.8%) to the proper group, and just 77 (25.2%) were misclassified.

With our new algorithm, we found a relevant improvement in the amount of cases that were correctly classified considering the breast cancer dataset and more cases were also correctly assigned to their group when the UCI datasets were analysed. For the breast cancer data, the number of patients which were assigned to their original class was 416 (38.8%), and 656 (61.2%) were wrongly classified. For the vehicle data, our method was able to properly classify 503 cases (59.5%), 122 more than with the naive Bayes. The remaining 343 instances (40.5%) were misclassified even with our new algorithm. When moving to the glass dataset, we obtained that 121 (56.5%) types were correctly assigned to their group, while the remaining 93 (43.5%) were not. The last dataset considered, haberman, had 240 (78.4%) data points properly classified and 66 (21.6%) misclassified.

When using a multinomial Logistic Regression model the number of cases correctly classified was higher with respect to previous techniques for the vehicle and glass data sets, but not for the breast cancer one. Concerning the haberman data, for which a GLM was fitted, we got the same results obtained with the naive Bayes classifier: a total of 229 (74.8%) patients were correctly assigned to their class, while the remaining 77 (25.2%) were not. A summary of our results is reported in Table 3. For the vehicle and glass datasets, average accuracies of different naive Bayes methods computed by Bouckaert [5] are also reported.

[Table 3 about here.]

From Table 3, it can be seen that our new algorithm outperformed the others in two sets of experiments (breast cancer and haberman data), while in the remaining two the MLR achieved the best accuracy. However, we were interested in developing an algorithm with a better performance than the traditional naive Bayes, and this goal was reached in all our tests. Comparisons of our method with black-box models like Neural Networks were out of the scope of this paper.

Calibration plots for the breast cancer, vehicle and glass data sets are reported in Fig. 3, 4, and 5. It can be seen that for the novel breast cancer dataset, the Logistic Regression model probabilities are less calibrated than for our new method. For the other data sets considered, Logistic Regression performed slightly better than our new algorithm.

[Figure 3 about here.]

[Figure 4 about here.]

[Figure 5 about here.]

As described in the experiment settings section, for the `haberman` data set a plot of the ROC curves for both the GLM and our method was produced and is reported in Fig. 6. From the values of the areas under the curves, reported in the plot, a slightly better accuracy of the GLM is evident with respect to our new method, which, in any case, seems to be a quite good predictive model for the `haberman` data.

[Figure 6 about here.]

6. Main contributions

From the results presented in the previous section, two different aspects may be highlighted: firstly, the new 'non-parametric' Bayesian classifier outperforms the traditional naive Bayes for all data sets considered, showing that the latter classifier is not suitable for problems where variables do not follow a normal distribution. Moreover, the similarity between our new approach and the naive Bayes one, in terms of algorithm structure, makes the 'non-parametric' method a white-box model. For someone not familiar with computational analysis it is easier to understand and interpret the set of classification rules derived from a white-box method.

We should also be aware of some disadvantages of the technique proposed in this work. If used with normal data, for example, the traditional naive Bayes classifier is likely to be more accurate than our method (results not shown). In addition, our proposed approach was developed to cope with continuous numerical data: its validation over mixed data sets remains open for future work.

7. Discussion and Conclusions

In this paper, we reviewed the naive Bayer classifier and applied it to four particular datasets. After a comparison between the Logistic Regression and the naive Bayes, we presented a new method for the implementation of a Bayesian classifier which deals with non-normal variables.

Over a novel breast cancer dataset and a set of benchmarks, we applied at the beginning the naive Bayes classifier, which is based on the assumption that numeric attributes follow a normal distribution. This method did not perform well on all data considered, and, if we focus on the `breast cancer` one, this reflects a sort of independence between biological markers and clinical information. Moreover, all our datasets' features strongly violated the normality assumption, thus suggesting that the naive Bayes might not be the most appropriate method to use.

Supervised learning techniques, like Neural Networks or Support Vector Machines, are widely used for classification purposes. Bayesian classifiers, like the naive Bayes, also continue to be popular learning algorithms for data mining applications due to their linear run-time [2]. However, in many real world problems, they are not very accurate.

To improve the naive Bayes performance, many different approaches have been proposed in literature [7, 8, 11]. Solutions like the Extended Naive Bayes [10] and the NB+ [12] are only two examples of techniques being validated over a number of data sets to show a better classification accuracy than the traditional naive Bayes. However, none of those methods tackled the issue of the non-normality of numerical continuous data. To solve this problem, we developed an algorithm similar to the naive Bayes but using a 'non-parametric' approach.

For each class and each variable, we computed the median value and the histogram of its distribution. We then considered different situations that might occur: if, fixing a particular class and a particular data point, the value of a generic variable was lower or greater than the extreme values of the same variable in the class considered at that stage, then we assigned a probability close to zero to that data point to belong to the specified class; if the value was identical to the median we set the probability to be one; finally, if the data point was smaller than the median, we calculated the area between the distribution's minimum and the actual value (or between the value and the distribution's maximum if value was greater than the median). We then divided the value obtained by half number of observations. As for the naive Bayesian classifier, we calculated, for each case, the product of probabilities of all features given the classes. We classified our data looking at the class number for which the above reached the maximum.

With the method just described, we were able to correctly classify a bigger amount of data points with respect to the naive Bayes, raising the percentage from 23.2% to 38.8% for the `breast cancer` dataset, from 45% to almost 60% for the `vehicle` Statlog dataset, from 48.6% to 56.5% for the `glass` data, and from almost 75% to more than 78% for the `haberman` dataset.

However, when using Logistic Regression, different results were obtained. For the `breast cancer` dataset, our model seemed to be more accurate (in terms of percentages of patients correctly classified) and more calibrated than the Logistic Regression. This was not true when considering the UCI data sets, for which our algorithm slightly appeared to be less calibrated and less accurate. However, for the `haberman` dataset, when a GLM was fitted to the data, the number of patients correctly assigned to their class was identical to the one obtained when using naive Bayes and the ROC curve associated to our method was very similar to the one produced by the GLM, providing two close values for the areas under the curve.

It is important to note that a couple of data sets presented in this work were also used in [5] to compare naive Bayes normal method with the kernel and the discretization ones obtaining both better and worse results compared to ours (Table 3). Bouckaert considered those three methods to deal with continuous variables when using the naive Bayes classifier. Instead our 'non-parametric' method was developed to deal with the non-normality of several dataset variables and, moreover, it outperformed all those proposed in [5] when applied over the `breast cancer` dataset (results not reported).

It is also worth noting that our developed method is not meant to be applicable over all available datasets. We have showed in this paper several situations for which a classical approach, the naive Bayes classifier, was outperformed by our more general algorithm that does not assume any particular distribution of the analysed features.

In conclusion, our proposed technique was more accurate than the traditional naive Bayes in all case studies analysed, without loosing the characteristics of a white-box model. However, its application over different types of data has not been investigated yet, leaving space for future research work.

Acknowledgements

This study was supported by the BIOPATTERN FP6 Network of Excellence (FP6-IST-508803) and the BIOPTRAIN FP6 Marie-Curie EST Fellowship (FP6-007597). Authors would also like to acknowledge the Turing Institute, Glasgow, Scotland for providing the `vehicle` Statlog dataset.

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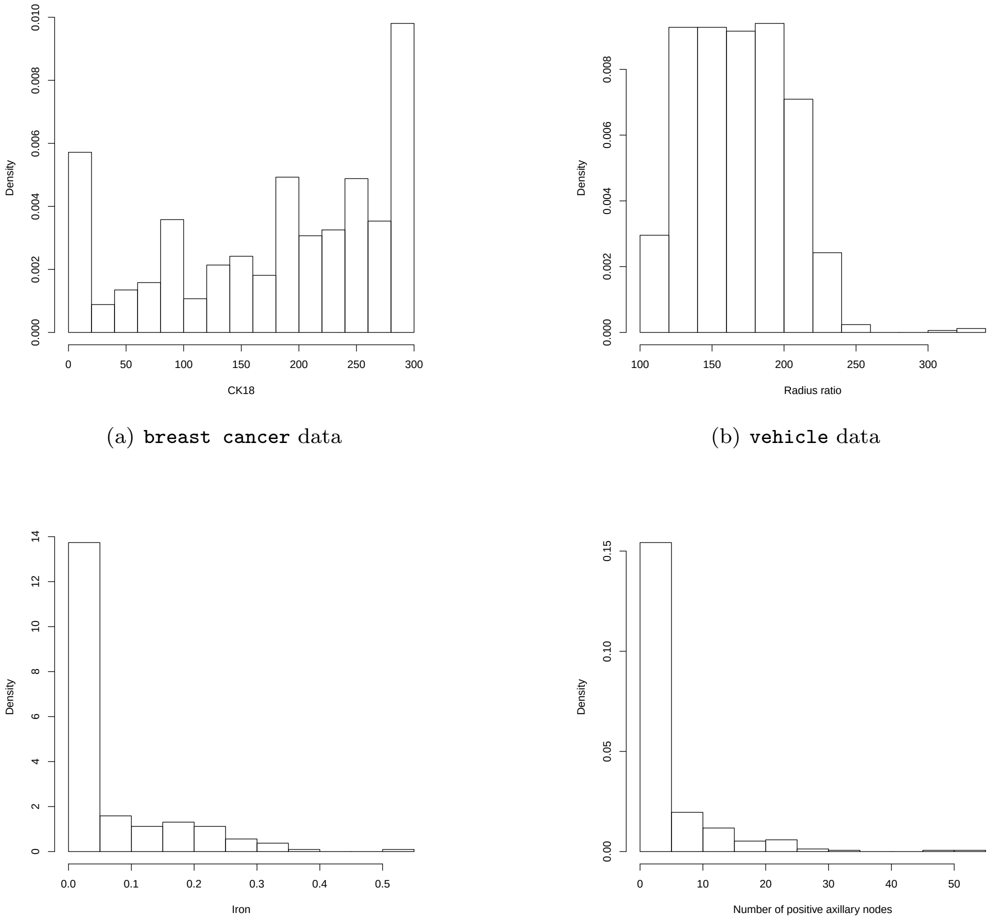


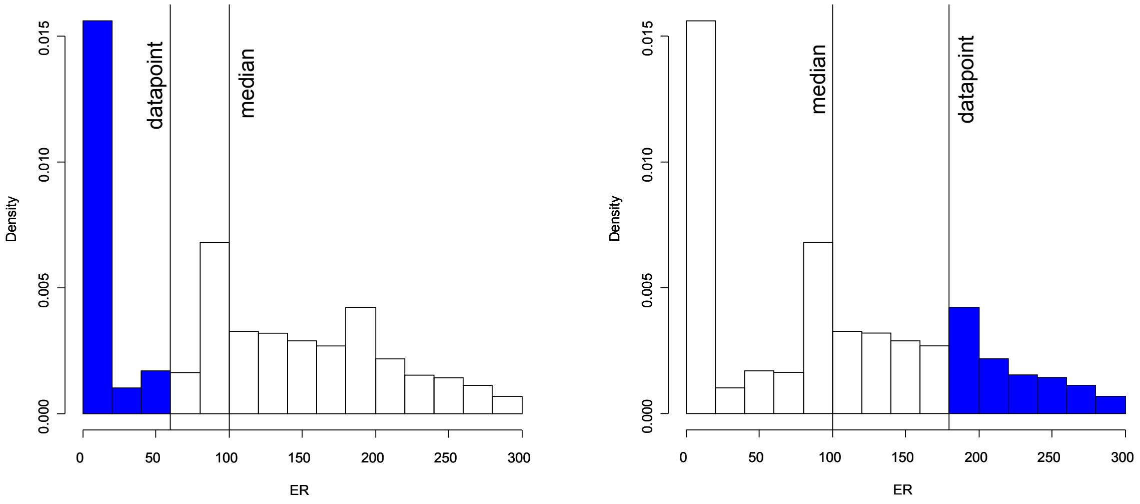
(a) `breast cancer` data

(b) `vehicle` data

(c) `glass` data

(d) `haberman` data

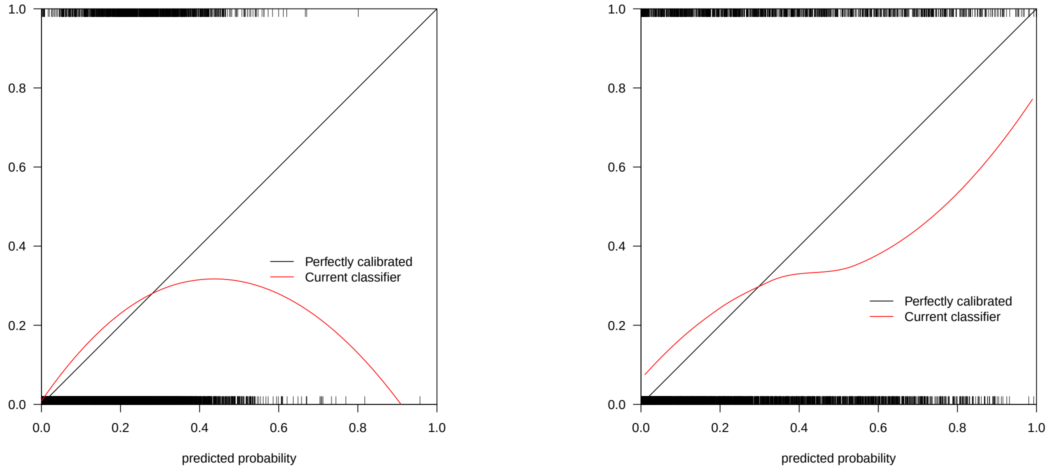
Figure 1: Histogram of sample variables



(a) If the value is smaller than the median

(b) If the value is bigger than the median

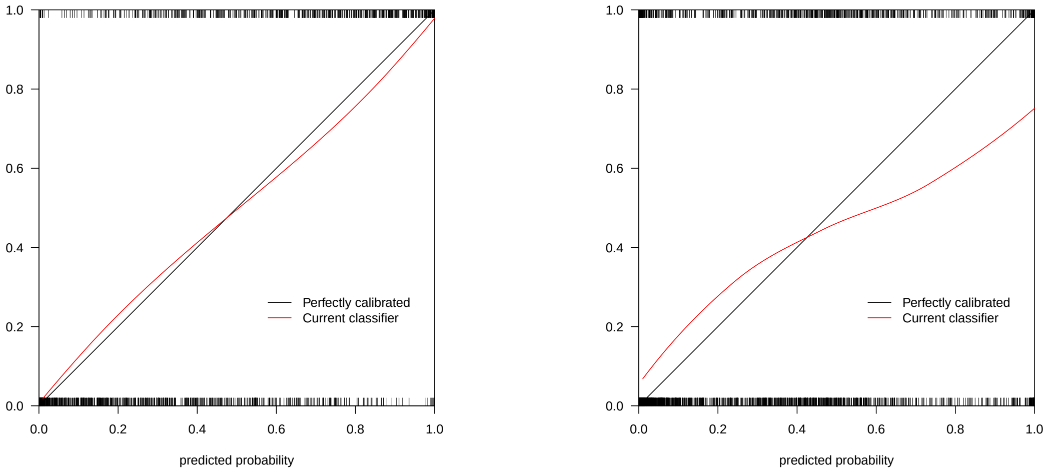
Figure 2: Area under the histogram



(a) MLR

(b) NPBC

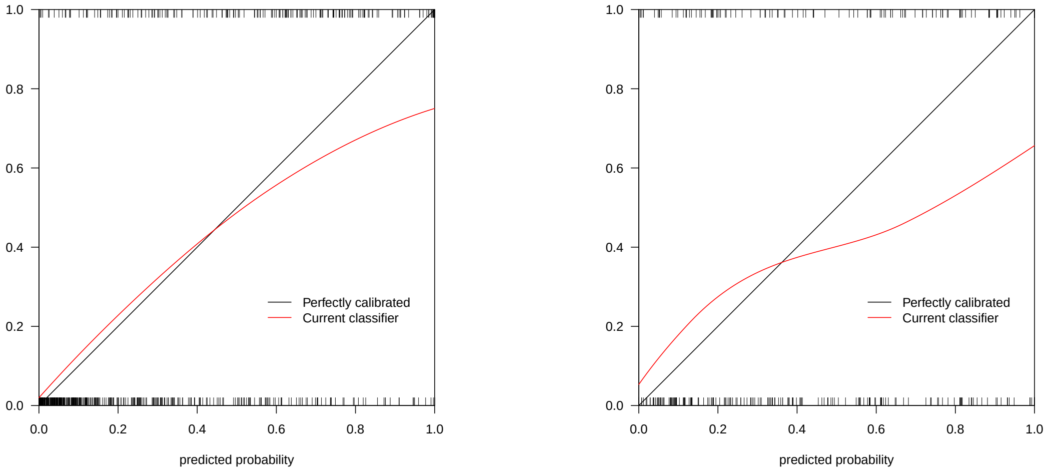
Figure 3: Calibration plots for multinomial logistic fit to the `breast cancer` data. MLR: Multinomial Logistic Regression, NPBC: Non-Parametric Bayesian Classifier



(a) MLR

(b) NPBC

Figure 4: Calibration plots for multinomial logistic fit to the `vehicle` data



(a) MLR

(b) NPBC

Figure 5: Calibration plots for multinomial logistic fit to the `glass` data

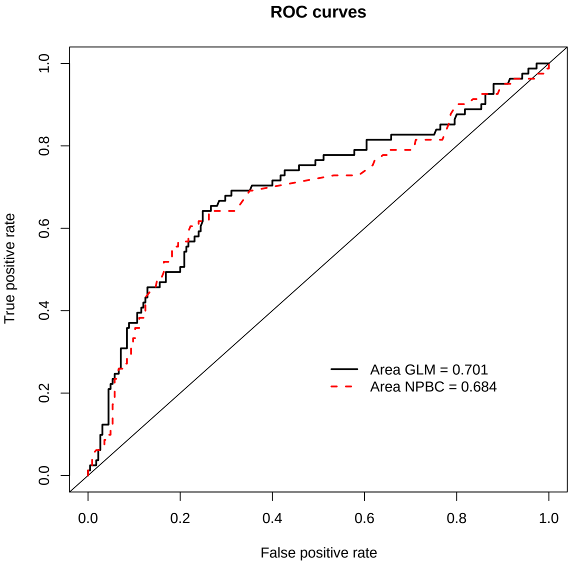


Figure 6: ROC curves for `haberman` survival data

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NPI Score	Prognostic Group
≤ 2.4	Excellent Prognostic Group (EPG)
2.5 - 3.4	Good Prognostic Group (GPG)
3.5 - 4.4	Moderate Prognostic Group 1 (MPG1)
4.5 - 5.4	Moderate Prognostic Group 2 (MPG2)
> 5.4	Poor Prognostic Group (PPG)

Table 1: NPI groups according to the value

name	breast_cancer	vehicle	glass	haberman
#pts	1076	846	214	306
#ats	25	18	9	3
#cls	5	4	6	2

#pts: the number of training data;

#ats: the number of attributes of patterns;

#cls: the number of classes.

Table 2: Summary of the datasets used ('breast cancer' plus three from UCI)

	breast_cancer		vehicle		glass		haberman	
Method	*Classified*	*Miscl.*	*Classified*	*Miscl.*	*Classified*	*Miscl.*	*Classified*	*Miscl.*
NB	249 (23.2%)	823	381 (45.0%)	465	104 (48.6%)	110	229 (74.8%)	77
MLR	332 (31.0%)	740	678 (80.1%)	168	134 (62.6%)	80	229 (74.8%)	77
BK [5]	—	—	(60.9%)	(39.1%)	(51.1%)	(48.9%)	—	—
BD [5]	—	—	(61.1%)	(38.9%)	(71.9%)	(28.1%)	—	—
NPBC	416 (38.8%)	656	503 (59.5%)	343	121 (56.5%)	93	240 (78.4%)	66

Table 3: Comparison of results. NB: Naive Bayes; MLR: Multinomial Logistic Regression; BK: Bouckaert's Kernel method; BD: Bouckaert's Discretisation method; NPBC: Non-Parametric Bayesian Classifier